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LLNL-TR-663216

# PRT/Sabbatical Report

J. G. Tobin

October 23, 2014

## Disclaimer

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# JG Tobin: PRT/Sabbatical Report **LLNL-TR-663216**

**Sabbatical Period:** October 1, 2013 to September 30, 2014, all of FY2014  
**Sabbatical Location:** Lawrence Berkeley National Laboratory, Berkeley, CA  
**Sabbatical Host:** David Shuh, Director of the Glenn T. Seaborg Center at LBNL

## **Runs at DOE User Facilities**

Sequoia Beamline, Spallation Neutron Source, ORNL, December 2013	Page 2
Beamline 8, Advanced Light Source, LBNL, February 2014	Page 4
Beamline 6-2, Stanford Synchrotron Radiation Lightsource, SLAC, March 2014	Page 6
Beamline 11-2, Stanford Synchrotron Radiation Lightsource, SLAC, April 2014	Page 7
Beamline 6-2, Stanford Synchrotron Radiation Lightsource, SLAC, June 2014	Page 6
Beamline 8, Advanced Light Source, LBNL, July 2014	Page 4

## **Conferences Organized**

AVS 60, Oct/Nov 2013, Long Beach, CA, Actinides and Rare Earth Sessions, Lead Org.  
Spring 2014 MRS, San Francisco, CA, Actinides Symposium, Head of Steering Comm.

## **Dedicated Volume on Actinide Core Level Spectroscopy, J. Electron Spectroscopy & Rel Ph.**

jgt co-editor	page 9
two articles with jgt as author	page 9
journal cover	page 9

## **Invited Talks** page 10

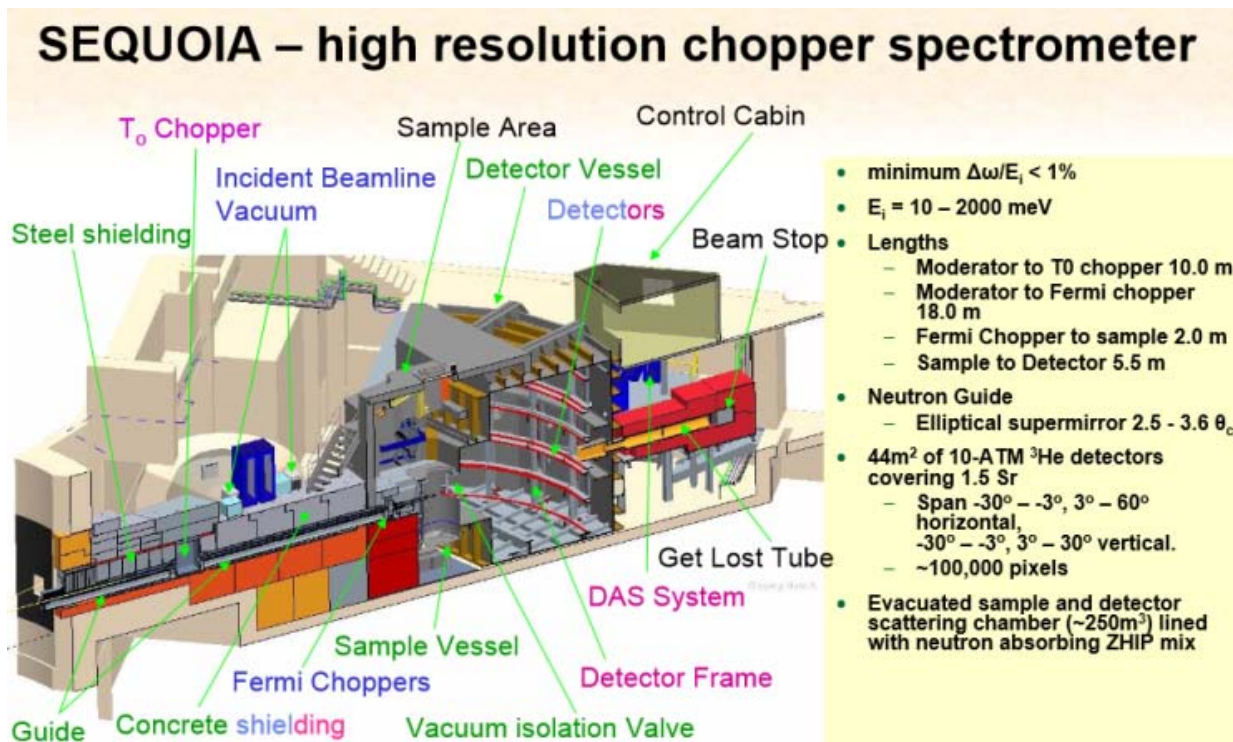
Spallation Neutron Source Seminar, ORNL, Oak Ridge, TN, December 2013  
American Chemical Society National Meeting, Dallas TX, March 2013  
Actinide XAS 2014, Paul Scherrer Institute, Boettstein, Switzerland  
Glenn T. Seaborg Center, LBNL, Berkeley, CA, June 2014  
Frontiers in Nuclear Science Lecture, PNNL, Richland, WA, July 2014  
Seaborg Institute Seminar, LANL, Los Alamos, NM, September 2014

Spallation Neutron Source, December 2013

Neutron Scattering Experiment upon CeNi: Looking for Electron Correlation in a Pu Surrogate



The Spallation Neutron Source is located at Oak Ridge National Laboratory in Tennessee. I travelled to ORNL to participate in the experiments. We used the Sequoia Facility at SNS to carry out our experiments.



This work was done under the auspices of our LLNL contract with the Russians. The leader of the experimental team was Alex Mirmelstein, from VNIITF in Snezhinsk, Russia. The other collaborators were from ORNL.

Our MRS Proceedings has already been published.

A.V. Mirmelstein, A. Podlesnyak, A.I. Kolesnikov, B. Saporov, A.S. Sefat, and JG Tobin,  
 “Neutron Scattering of CeNi at the SNS-ORNL: A Preliminary Report,”

Matl. Res. Soc. Symp. Proc. **1683**, s08-02 (2014), DOI: <http://dx.doi.org/10.1557/opl.2014.432>.



LLNL-PROC-649216

## Neutron Scattering of CeNi at the Spallation Neutron Source at Oak Ridge National Laboratory: A Preliminary Report

J. G. Tobin, A. V. Mirmelstein, A. Podlesnyak, A. I. Kolesnikov

January 29, 2014

MRS Spring 2014  
 San Francisco, CA, United States  
 April 20, 2013 through April 25, 2014

### Neutron Scattering of CeNi at the SNS-ORNL: A Preliminary Report

A.V. Mirmelstein<sup>1</sup>, A. Podlesnyak<sup>2</sup>, A.I. Kolesnikov<sup>3</sup>, and JG Tobin<sup>4</sup>  
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<sup>2</sup>Quantum Condensed Matter Div., Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA  
<sup>3</sup>Neutron Scattering Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN USA,  
<sup>4</sup>Lawrence Livermore National Laboratory, Livermore, CA, USA 94550.

#### ABSTRACT

This is a preliminary report of a neutron scattering experiment used to investigate 4f electron behavior in Ce.

#### INTRODUCTION

The manifestations of electron-correlation in Pu and Ce have interesting parallels [1], including large volume collapses between phases. [2-3] CeNi, using Ni 60 to minimize the Ni magnetic scattering [4], was chosen as an avenue to probe the magnetic cancellation in Ce. This magnetic cancellation should be of the Kondo type, with the valence electrons screening the f electron moment. [5-7] This screening should change under pressure. [8,9] The neutron scattering experiments [10] were carried out at the Spallation Neutron Source [11] at Oak Ridge National Laboratory, using the Sequoia Facility. [12]

#### EXPERIMENT AND DISCUSSION

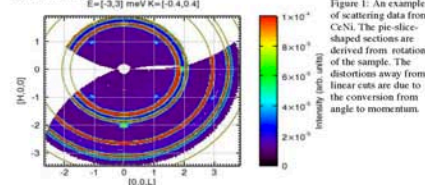


Figure 1: An example of scattering data from CeNi. The pie-slice-shaped sections are derived from rotation of the sample. The distortions away from linear cuts are due to the conversion from angle to momentum.

Pulsed neutrons are generated by the acceleration of protons into a target. The pulsed neutron beams are scattered off of the samples in various beam-lines. In the Sequoia Beam-line, a large area, position sensitive detector collects the scattered neutrons. Energy analysis comes from time-of-flight, momentum from the combination of energy and angle in the position sensitive detector. Thus, the data collection is four dimensional: energy and three components of momentum. The sample can also be rotated about a vertical axis, permitting different angles of incidence. Data analysis involves summing over various angles and energies, providing cuts through the multi-dimensional data space, to permit 2-D and 3-D plots. An example is shown in Figure 1. This data can then be symmetrized, an example of which is shown in Figure 2.

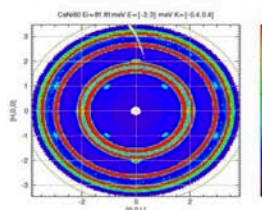


Figure 2: Scattering Data. The bright red and green rings are powder patterns from the polycrystalline Al of the pressure vessel. The individual spots are from the single-crystal CeNi.

It is the energy loss that will provide a measure of the electron correlation. (Figure 3) The data shown here is all at ambient pressure. Measurements at 400 bar, 800 bar and 2200 bar suggest changes in the energy loss spectra. A sophisticated subtraction of the Al background must be done prior to a full analysis.

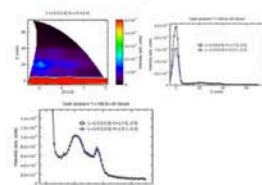


Figure 3: Data reduction to look at energy loss. Top left: Isolating a Bragg scattering peak of CeNi. Top right: Comparing the Bragg scattering peaks and energy loss for two peaks. Bottom: Blow-up of the comparison of the energy loss of two Bragg scattering peaks. The top label represents that the sample is CeNi in an Al sample holder.

#### ACKNOWLEDGMENTS

Lawrence Livermore National Laboratory is operated by Lawrence Livermore National Security, LLC, for the U.S. Department of Energy, National Nuclear Security Administration under Contract No. DE-AC52-07NA27344. Work at VNIITP was supported in part by Contract B601122 between LLNL and VNIITP. The Spallation Neutron Source and Oak Ridge National Laboratory are supported by the DOE Office of Science, Office of Basic Energy Science.

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12. G. E. Granroth, A. I. Kolesnikov, T. E. Shorline, J. P. Clancy, K.A. Ross, J. P. C. Ruff, B. D. Gaulin, S. E. Nagler, *J. Phys.: Conf. Series* **251**, 012058 (2010).

## ALS Soft X-ray Experiments

Sample Transfer and Mounting in the Heavy Element Radiological Laboratory (HERL) at LBNL



Here I am in the HERL with David Shuh (not shown).



UF<sub>4</sub> was shipped in a plastic box inside a stainless steel can from LLNL.



UF<sub>4</sub> sample sitting in plastic box after being unwrapped.



ALS Transport container on lab bench.



UF<sub>4</sub> (blue-green) sitting on the adhesive carbon strips on the sample platen. The work was performed by DKS in a lab on the first floor of B70A, with assistance by me. The sample platen was from BL8, for the Soft X-ray Fluorescence (SXF) spectrometer. The plate is about 1 inch long.



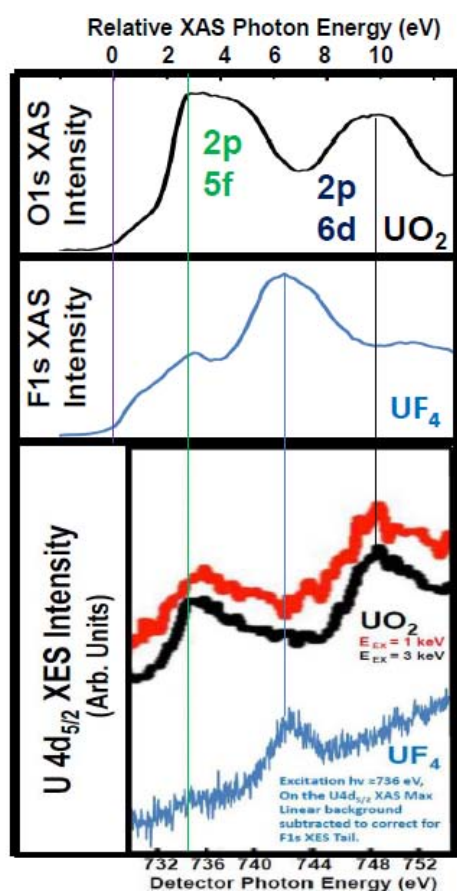
Mounted UF<sub>4</sub> sample in vessel for transport to ALS.



February and June 2014

Synchrotron Radiation Beamtime at Beamline 8 at the Advanced Light Source (ALS) at LBNL

Soft X-ray Absorption and Emission as a probe of covalency in  $\text{UO}_2$  and  $\text{UF}_4$



An important issue which has arisen recently is the question of the role of covalency in the actinide oxides. Building upon our earlier PRL in 2011, we are extending our investigations to  $\text{UF}_4$ . In terms of formal charge, the U should be +4 in each of these compounds. However, F is a stronger oxidizing agent and should exhibit less covalency and more ionicity than the  $\text{UO}_2$ . The XAS K Edge (O1s and F1s) allow us to probe the oxidant 2p contribution to the bond. The U 4d XES is a window to the U 5f contribution.

Our new measurements upon  $\text{UF}_4$ , shown to the left and compared with the results for  $\text{UO}_2$ , support this contention. Hence, we have opened the door to directly probing covalency in actinide oxides, fluorides and other compounds with these measurements. (I collected this data with Ruimin Qiao of the ALS.)

## Synchrotron Radiation Beamtime at Beamline 6-2 at the Stanford Synchrotron Light Source (SSRL)

Hard X-ray Absorption and Emission as a probe of covalency in  $\text{UO}_2$  and  $\text{UF}_4$ 

## SSRL Gains New Spectrometry Capabilities

A new spectroscopy instrument has been installed on Beamline 6-2 at the Stanford Synchrotron Radiation Lightsource, where staff scientists are now working to test its various components before offering beam time to users this spring. The setup will expand SSRL capabilities in X-ray Raman and X-ray emission spectroscopy—two techniques used to analyze the organization of electrons in solids, liquids and gases—and keep SSRL positioned as a leading synchrotron user facility.

"This will open up the science to a whole new set of users," said SSRL staff scientist Dennis Nordlund, who is part of the team building the instrument. According to Nordlund, the higher intensity and better resolution offered by the X-ray Raman instrument make it a very competitive alternative to soft X-ray spectroscopy. What's more, he says, it overcomes many technical limitations that come with soft X-ray studies, such as the need to operate under a vacuum.



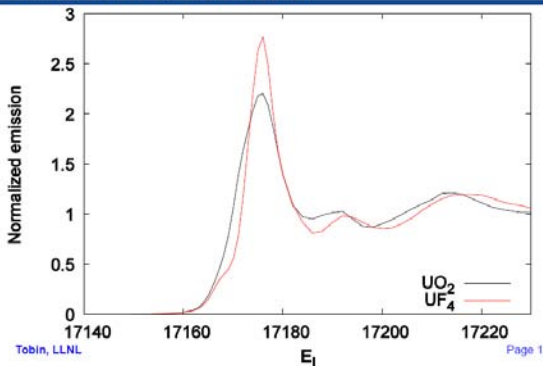
Dimosthenis Sokaras at SSRL Beamline 6-2. (Photo by Brad Plummer.)

We have made use of the new facilities at BL 6-2 to carry out Resonant X-ray Emission Spectroscopy of actinides. (I collected this data with Corwin Booth of LBNL, with the assistance of the SSRL Beamline Scientists Dimos Sokaras and Tsu Chien Weng.)

Comparison of UL3 XAS-PFY for  $\text{UO}_2$  and  $\text{UF}_4$  22March2014

Excitation Photons near UL3 Edge (17.2 keV)

Detection Photons near U L-alpha 1(13.6 keV)



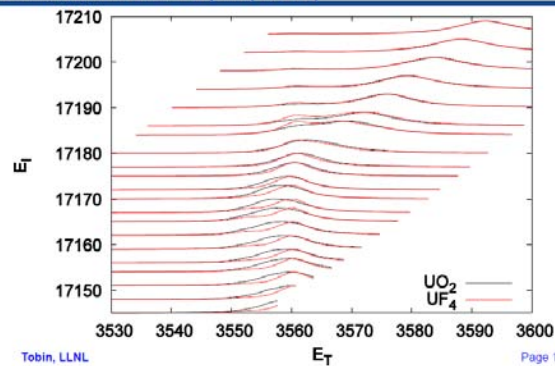
Tobin, LLNL

Page 1

Comparison of RXES for  $\text{UO}_2$  and  $\text{UF}_4$  21March2014

Excitation Photons near UL3 Edge (17.2 keV)

Detection Photons near U L-alpha 1(13.6 keV)



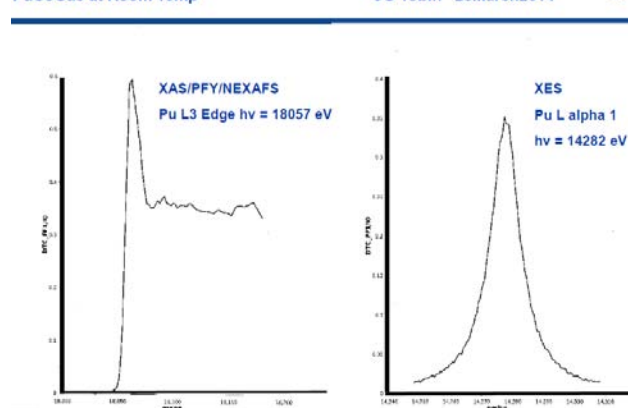
Tobin, LLNL

Page 1

Pu X-ray Absorption and X-ray Emission Spectroscopy: BL6-2 at SSRL

PuCoGa5 at Room Temp

JG Tobin 25March2014



Above is a comparison of the results for  $\text{UO}_2$  and  $\text{UF}_4$ , illustrating the narrowing associated with the more ionic  $\text{UF}_4$ . While the broadening in the  $\text{UO}_2$  relative to the  $\text{UF}_4$  can be shown to be driven by ligand field symmetry effects, it is possible that covalency is closely related to the broadening.

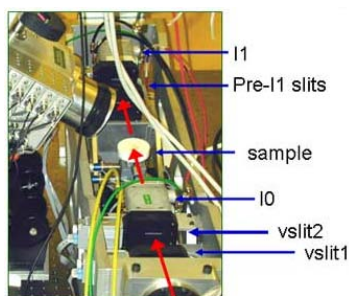
To the left is some Pu L3 edge data. We also worked on some Pu compounds.



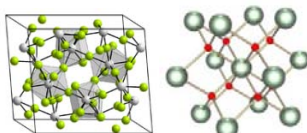
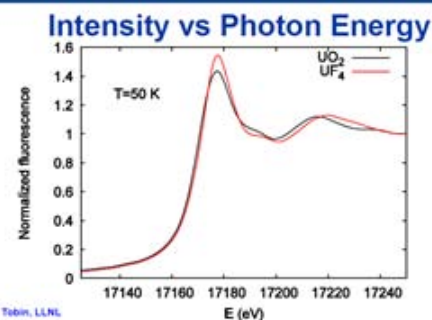
## Synchrotron Radiation Beamtime at Beamline 11-2 at the Stanford Synchrotron Light Source (SSRL)

Hard X-ray Absorption, XANES and EXAFS, as a probe of covalency in  $\text{UO}_2$  and  $\text{UF}_4$ 

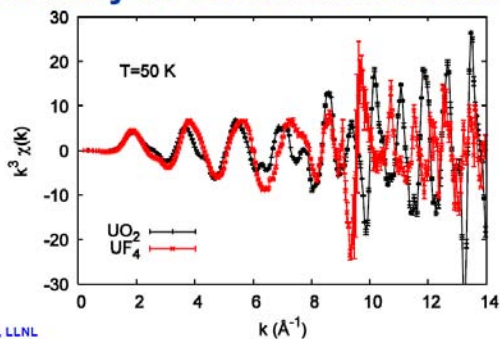
Beam Line 11-2 is a high-flux XAS station dedicated to molecular biogeochemical and interface sciences. It is optimized for challenging XAS measurements on dilute or radioactive samples, single crystals, and interfaces. To support these experiments, Beam Line 11-2 is equipped with collimating and focusing optics, a "double double" Si(220) LN-cooled monochromator, and a 30-element solid state Ge detector array. Additional instrumentation includes LHe and LN cryostats, a grazing incidence XAS spectrometer, and HEPA-filtered controlled exhaust systems that are continuously monitored to detect the presence of air-borne radioactivity. It has an adjacent sample preparation room for handling and temporary storage of radioactive samples, most of which are related to the DOE's energy and national security missions.



The beamline setup.

Left:  $\text{UF}_4$  is monoclinic.Right:  $\text{UO}_2$  is a fluorite (cubic) structureU L3 XANES for  $\text{UF}_4$  and  $\text{UO}_2$  from BL11-2, Apr2014  
XANES = X-ray Absorption Near Edge StructureU L3 EXAFS for  $\text{UF}_4$  and  $\text{UO}_2$  from BL11-2, Apr2014  
EXAFS = Extended X-ray Absorption Fine Structure

## Intensity vs Electron Momentum

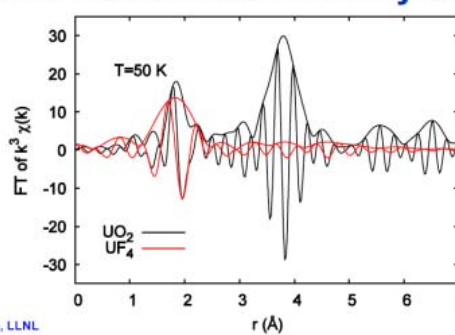


Tobin, LLNL

Page 2

U L3 EXAFS for  $\text{UF}_4$  and  $\text{UO}_2$  from BL11-2, Apr2014  
EXAFS = Extended X-ray Absorption Fine Structure

## Fourier Transform Intensity vs r (Å)



Tobin, LLNL

Page 3

XANES is a measure of the unoccupied electronic structure. EXAFS provides information about nearby scatterers and thus bond lengths. Corwin Booth and I collected this data on BL 11-2 in April 2014.

Here are some BL 11-2 results from a Pu system.



LLNL-TR-657137

## Summary of EXAFS results on Cd-doped PuRhIn5

C. H. Booth, E. D. Bauer, J. G. Tobin

July 15, 2014

### Summary of EXAFS results on Cd-doped PuRhIn5

C. H. Booth  
Chemical Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, California 94720, USA\*

E. D. Bauer  
Materials Physics and Applications Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA

J. G. Tobin  
Lawrence Livermore National Laboratory  
(Dated: June 11, 2014)

Extended x-ray absorption fine-structure (EXAFS) data of a solid sample of PuRhIn<sub>5</sub> and a ~2% Cd-doped PuRhIn<sub>5</sub> were obtained in fluorescence mode from the Pu L<sub>2,3</sub> and the Rh, In, and Cd K edges. Pu-edge results are consistent with the known structure PuRhIn<sub>5</sub> for both samples. Rh-edge results are also consistent with the nominal crystal structure, but indicate some Rh in impurity phase in the Cd-doped sample. In-edge fits fit the nominal structure well, and are not as sensitive to the possible impurity. Cd-edge data were used to determine how much of the Cd resides on In(1) sites, and we find 49% ± 5% substitute for Cd onto the In(1) site, in contrast to the 20% one would expect by a random distribution of Cd onto both the In(1) and In(2) sites. This result is consistent with similar data on CeCoIn<sub>5</sub> doped with Cd reported previously.

#### I. INTRODUCTION

The crystal structure of PuRhIn<sub>5</sub> is shown in Fig. 1.

#### II. EXPERIMENTAL DETAILS

A Cd-doped sample and a control sample of PuRhIn<sub>5</sub> were prepared. The Cd concentration of between 1% and 2% was determined by (microprobe/72) on samples that started from similar nominal Cd concentrations. X-ray diffraction... Magnetic susceptibility...

EXAFS data were collected at 30 K from the Pu L<sub>2,3</sub> edge and at 50 K from the Rh, In, and Cd edges using a Si(220) (α = 0°) half-tuned double monochromator on BL 11-2 at the Stanford Synchrotron Radiation Light-

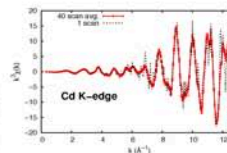


FIG. 2: (Color online) Cd K-edge EXAFS data at 50 K.

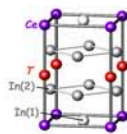


FIG. 1: (Color online) The tetragonal unit cell of the Ce115s.

\*Electronic address: cthooth@lbl.gov

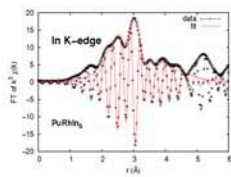


FIG. 3: (Color online) In K-edge EXAFS data (points) and fit (line) in r-space after Fourier transform (FT) of the k-space data from 2.5-13.0 Å⁻¹. Gaussian narrowed by 0.3 Å⁻¹. These data were fit between 1.9 and 5.1 Å to a model described in the text and more fully in Ref. 6. Error bars are determined from multiple scans and indicate reproducibility.

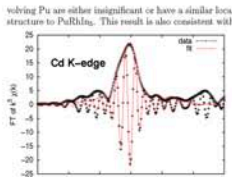


FIG. 4: (Color online) Cd K-edge EXAFS data (points) and fit (line) in r-space, as described in Fig. 3. The resulting fit parameters are described in Table I.

differentiate between In and Cd as backscattering atoms. Instead, the most important data is that from the Cd edge, since different bond lengths are expected depending on whether the Cd sits on the In(1) or the In(2) site. The In edge data are used as a check for the heavily-constrained fitting model.

Although the differences in the local structure between the In(1) and In(2) sites are significant, even in the nominal crystal structure there are many distinct scattering paths, potentially generating more fit parameters than can be reasonably fit. We therefore employ a fit model that includes many constraints, as previously used on Cd-doped CeCoIn<sub>5</sub> [6]. Within this model, there are only three fit parameters that determine all the bond lengths, many of the Debye-Waller factors (σ²) are either constrained to similar scattering pairs or simply held fixed, and a single E<sub>0</sub> threshold shift is employed, as well as a single amplitude reduction factor S<sub>0</sub>². In this way, the fit model can include 20 single scattering paths up to 7 Å, including the Cd backscattering atoms, while only allowing 10 fit parameters to vary in the Cd K-edge case. The data were fit in r-space between 1.9 and 5.1 Å after being Fourier transformed between 2.5 and 13.0 Å⁻¹ (Gaussian narrowed by 0.3 Å⁻¹). The fit degrees of freedom were determined to be 13.4 [7].

#### III. RESULTS

The Pu L<sub>2,3</sub>-edge EXAFS from both samples were found to be consistent with the nominal crystal structure, indicating that any potential impurity phase in-

volving Pu are either insignificant or have a similar local structure to PuRhIn<sub>5</sub>. This result is also consistent with the relatively large magnetic moment of 0.9 μ<sub>B</sub>. Likewise, Rh edge data from PuRhIn<sub>5</sub> are consistent with the nominal crystal structure; however, a reduction in amplitude on such data from PuRhIn<sub>5</sub>Cd may indicate a Rh/In impurity phase, possibly RhIn<sub>3</sub>. From the amplitude reduction and comparing to FEFF [1] simulations on PuRhIn<sub>5</sub> and RhIn<sub>3</sub>, we estimate a maximum RhIn<sub>3</sub> impurity of 15%. Such a reduction would cause only a maximum ~7% error in the susceptibility, and so is likely insignificant for the present results.

Fits to the In K-edge data (Fig. 3) indicate the fitting model is reasonably accurate, giving a fraction *f* of In on the In(1) site of 20% ± 7%, compared to the nominal crystal structure value of 20% in on the In(1) site.

The main result of this work stems from the fits to the Cd K-edge data, shown in Fig. 4. The fit parameters are summarized in Table I. In particular, these fits indicate *f* = 49% ± 5%, very much like that found previously in Cd-doped CeCoIn<sub>5</sub> [6].

#### Acknowledgments

Supported by the U.S. Department of Energy (DOE) under Contract No. DE-AC02-02CH11201 (Lawrence Berkeley National Laboratory) and further supported by the U.S. DOE (Los Alamos). X-ray absorption data were collected at the Stanford Synchrotron Radiation Lightsource, a national user facility operated by Stanford University on behalf of the DOE, Office of Basic Energy Sciences.

TABLE I. Fit results from Cd K-edge fit range is between 1.90 and 5.10 Å. The k<sup>-1</sup>-weighted data are transformed between 2.50-13.00 Å⁻¹ and are Gaussian narrowed by 0.30 Å⁻¹. Fit assumes 2 at% Cd concentration.

	<i>N</i>	<i>σ</i> <sup>2</sup> (Å <sup>2</sup> )	<i>R</i> (%)
Cd1 Pu3.2675 f	1.02	0.0004(18)	3.23(2)
Cd1 In3.2796 f	2.76	0.0007(9)	3.18(1)
Cd1 Cd2.3276 f	0.08	0.00009	3.180
Cd1 In1.4620 f	1.88	0.01000	4.606
Cd1 Cd1.4620 f	0.04	0.01000	4.606
Cd1 Rh1.4958 f	3.84	0.011(8)	4.089
Cd2 In3.2702 f	1.04	0.000(3)	2.92(2)
Cd2 In1.4651 f	0.51	0.01000	3.149
Cd2 Cd2.2801 f	0.01	0.01000	3.149
Cd2 In3.2673 f	2.04	0.00009	3.320
Cd2 Cd2.3267 f	0.04	0.00000	3.320
Cd2 Pu3.2796 f	1.04	0.00040	3.180
Cd2 In3.2796 f	1.02	0.00009	3.180
Cd2 Cd1.3276 f	0.02	0.00009	3.180
Cd2 In1.4603 f	2.04	0.000(2)	4.573
Cd2 Cd2.4363 f	0.04	0.00310	4.573
Cd2 In1.4607 f	2.04	0.01000	4.606
Cd2 Cd2.4620 f	0.04	0.01000	4.606
Cd2 In1.4652 f	0.51	0.01000	4.302
Cd2 Cd2.4652 f	0.01	0.01000	4.302
ΔE <sub>0</sub>		-8.9(33)	
S <sub>0</sub> ²		1.000	
<i>f</i>		0.490(40)	
<i>R</i> (%)		13.60	

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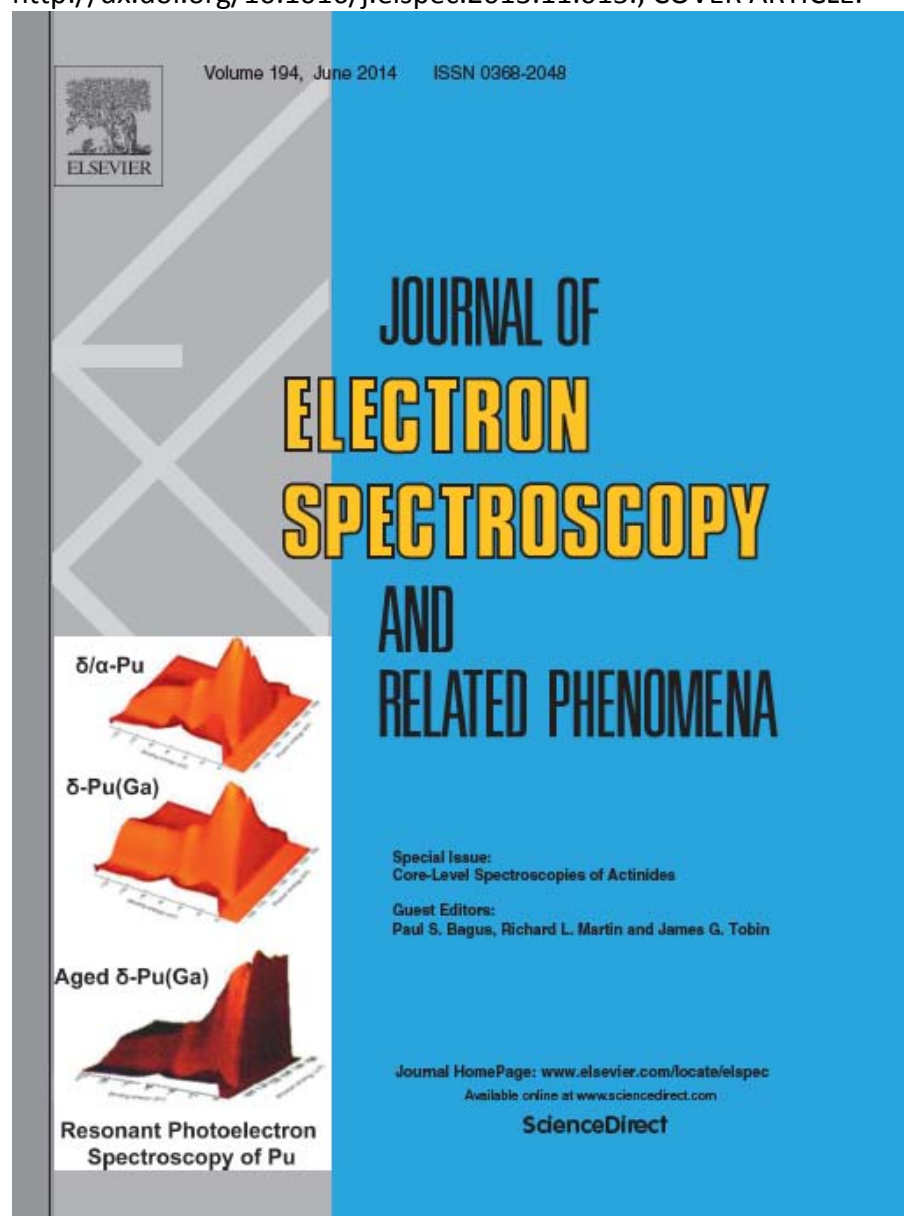
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**Dedicated Volume on Actinide Core Level Spectroscopy  
Editorship**

P. Bagus, R.L. Martin, and J.G. Tobin, ed., Actinide Core Level Spectroscopy and Electronic Structure," J. Electron Spectroscopy and Rel. Phen., **194**, 1 (2014); <http://dx.doi.org/10.1016/j.elspec.2014.05.006>.

**Refereed Publications**

1. J.G. Tobin, "The apparent absence of chemical sensitivity in the X-ray absorption spectroscopy of uranium compounds," J. Electron Spectroscopy and Rel. Phen., **194**, 14 (2014); <http://dx.doi.org/10.1016/j.elspec.2014.01.020>.
2. M.V. Ryzhkov, A. Mirmelstein, B. Delley, S.-W. Yu, B.W. Chung, J.G. Tobin, "The Effects of Mesoscale Confinement in Pu Clusters," J. Electron Spectroscopy and Rel. Phen., **194**, 45 (2014); <http://dx.doi.org/10.1016/j.elspec.2013.11.015>, COVER ARTICLE.



## Invited Talks

1. JG Tobin, "Soft X-ray Spectroscopy of the Actinides," Spallation Neutron Source Seminar, Oak Ridge National Laboratory, Oak Ridge, TN, December 12, 2013.
2. JG Tobin, "The Absence of Chemical Sensitivity in the 4d and 5d X-ray Absorption Spectroscopy of Uranium Compounds," Norman Edelstein Award Sessions, ACS National Meeting, Dallas, TX, March 2014.
3. JG Tobin, "Evolution in Pu Nanocluster Electronic Structure: From Atomicity to 3-D," ACS National Meeting, Dallas, TX, March 2014.
4. JG Tobin, "The Absence of Chemical Sensitivity in the 4d and 5d X-ray Absorption Spectroscopy of Uranium Compounds and How To Get Around It," Actinide XAS 2014, Paul Scherrer Institute, Schloss Boettstein, Boettstein, Switzerland, May 2014.
5. JG Tobin, "Resolving the Issues of 5f Covalency and Ionicity in UO<sub>2</sub> and UF<sub>4</sub>," Glenn T. Seaborg Center Seminar, Lawrence Berkeley National Laboratory, Berkeley, CA, June 11, 2014.
6. JG Tobin, "Resolving the Issues of 5f Covalency and Ionicity in UO<sub>2</sub> and UF<sub>4</sub>," Frontiers in Nuclear Science Lecture Series, Pacific Northwest National Laboratory, Richland, WA, July 24, 2014.
7. JG Tobin, "Resolving the Issues of 5f Covalency and Ionicity in UO<sub>2</sub> and UF<sub>4</sub>," Seaborg Institute Seminar, Los Alamos National Laboratory, Los Alamos, NM, September 24, 2014.